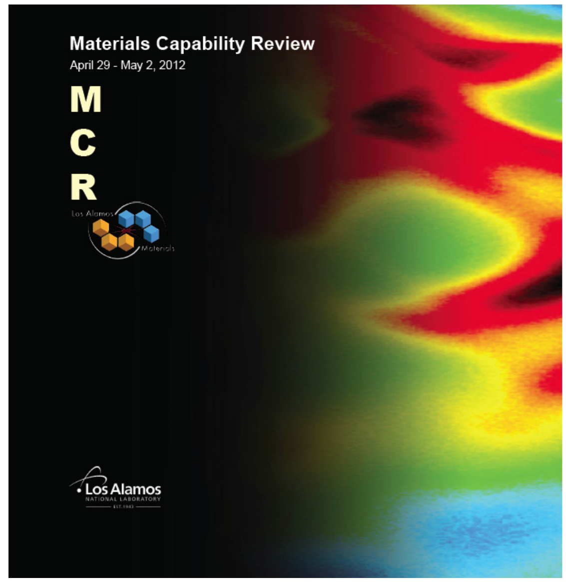
MPA MaterialsMatter

April 2012

INSIDE

Laboratory's materials research to be showcased at capability review



The world-record highest non-destructive magnetic field achieved last month at the National High Magnetic Field Laboratory-Pulsed Field Facility (see article, page 4) will be just one technical achievement featured during the 2012 Materials Capability Review.

From April 29 to May 2 scientists from 18 groups and 8 divisions will discuss their research in presentation and poster sessions at the Oppenheimer Study Center and the National High Magnetic Field Laboratory.

Organized by the Experimental Physical Sciences Directorate, the external peer review is designed to assess the quality of materials research and provide advice on technical contributions. This year's review will emphasize research in computational co-design for materials; high explosives and high pressure; high magnetic fields; and condensed matter physics.

Technical sessions begin Monday, April 30 at 8:30 a.m. when the review's technical host Materials Physics and Applications Division Leader Toni Taylor will present an overview of Materials at Los Alamos, including an update on an implementation plan for the Materials Strategy. She will be followed by MaRIE Capture Manager John Sarrao, who will discuss the latest developments related to the Laboratory's proposed flagship experimental facility for predicting and controlling materials in dynamic extremes.

For the 2012 Materials Capability Review, Gary Was of the University of Michigan returns to co-chair, with Barbara Jones of IBM Research-Almaden, a nine-member committee from universities, national laboratories, and research institutions. Theme leaders are Theoretical Division Leader Antonio Redondo, Weapons Experiments Division Leader David Funk, NHMFL-PFF Director Charles Mielke, and Condensed Matter & Magnet Science Group Leader Michael Hundley.

Members of the Laboratory's materials community are invited to attend.The agenda will be available on the internal ADEPS home page at int.lanl.gov/org/padste/adeps/.

MPA MaterialsMatter

From David's Desk

The Materials Capability Review, highlighted on the cover of this newsletter, is an important annual assessment of the status of materials science across LANL. Toni and I encourage you to attend the review. It is a good opportunity to hear about some of the most significant achievements of your colleagues, and to gain a broader understanding of the materials capability. Use this event to inform yourself and strengthen the connections of your research interests to our materials strategy.

From a strategic perspective, now is a good time to address the impact of the Voluntary Separation Plan on MPA Division, and to address other issues relevant to the long-term vitality of the Division. Only two individuals took the VSP in MPA Division: Ian Campbell from MPA-11 and Jose (Ernie) Serna from MPA-CMMS. The work these individuals did remains important to the Division and the Laboratory, but we have personnel with the skills to continue the efforts. Nevertheless, we will miss them and wish them well.

The impact of the VSP on the ability of the Laboratory to execute its programs will be significant, and the Laboratory budget for FY-12 remains tight. The Nuclear Weapons budget remains the biggest concern for the Laboratory. For MPA Division the bigger problems are the increase in overhead to cover the VSP as well as other institutional expenses. This will likely exacerbate tight budgets in areas where our position was weak this fiscal year. Applied Energy programs are the most likely to suffer, although all of our efforts will be adversely affected.

In addition, you can expect that personnel reductions and changes in job assignments will continue to create some issues for anything from proposal preparation to facility maintenance. For example, we heard that the annual deadlines for submitting large purchase orders will be earlier this year, so that the personnel engaged in the process have more time to do the job. Organizations are working to backfill positions and ensure that critical jobs are covered, but this is a complicated task. Your patience and understanding will be appreciated.

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As we look to the future, MPA remains a vital organization with an entrepreneurial spirit that is at the core of our successes. Obtaining funding for some areas of research is becoming more challenging, but new opportunities are also on the horizon. MPA-DO, in concert with other divisions and program office personnel, has been working to find ways to engage in the new critical materials initiative out of DOE. Talk to your group leader if you have technical ideas that might apply. In addition, we are closely following the new mesoscale materials initiative. Many of you have supplied ideas for important mesoscale science, and while it may be a year before any call comes out, now is the time to put forth concepts that might influence the research objectives of this new initiative and also lay the groundwork for how LANL might respond.

Finally, we have been working on facility planning for the long term. As the Laboratory works on revitalizing the research campus, it is our goal to optimize the plan so that new buildings facilitate implementing the materials strategic plan. The MSL infill project is the first of these efforts, but we are optimistic we can consolidate more of our organization around the materials complex in facilities that position us for future programmatic work.

MPA Deputy Division Leader David Watkins

Nathan Mara to receive TMS Young Leaders Professional Development Award

The Minerals, Metals and Materials Society (TMS) has selected Nathan Mara (Center for Integrated Nanotechnologies, MPA-CINT) to receive the 2012 TMS Materials Processing and Manufacturing Division Young Leader Professional Development Award. The Society created the annual award to enhance the professional development of dynamic young people from TMS's five technical divisions. Awardees participate in Society activities, attend TMS conferences, network with Society members and leaders, receive mentoring from TMS division leaders, and serve as judges for division-sponsored student events at the TMS Annual Meeting.

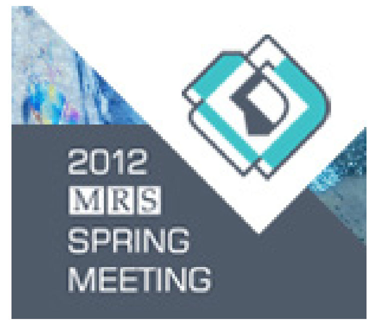
Mara earned his doctorate at the University of California, Davis. In 2005, he joined CINT as a Director's Postdoctoral Fellow, where he examined plastic flow behavior in laminar nanocomposites. Since 2008, Mara has been a staff scientist in MPA-CINT and Metallurgy (MST-6). His research interests include the synthesis of bulk structural nanocomposites and interfacial effects on material performance at mechanical and radiation extremes. Mara is the nanomechanical testing subject matter expert at CINT, the experimental project lead for the mechanical behaviors thrust in the Center for Materials at Irradiation and Mechanical Extremes (CMIME), and the experimental team lead for the Laboratory Directed Research and Development (LDRD) project "Innovative and Validated Sub-micron to Mesoscale Modeling of the Evolution of Interface Structure and Properties under Extreme Strains." Mara received the 2010 LANL Distinguished Mentor Performance Award for leading small teams of students, postdoctoral researchers, and staff.

The Minerals, Metals & Materials Society (TMS) is an international professional organization of nearly 10,000 members, encompassing the entire range of materials and engineering, from minerals processing and primary metals production to basic research and the advanced applications of materials.

LANL organizes and sponsors actinide symposium at MRS conference

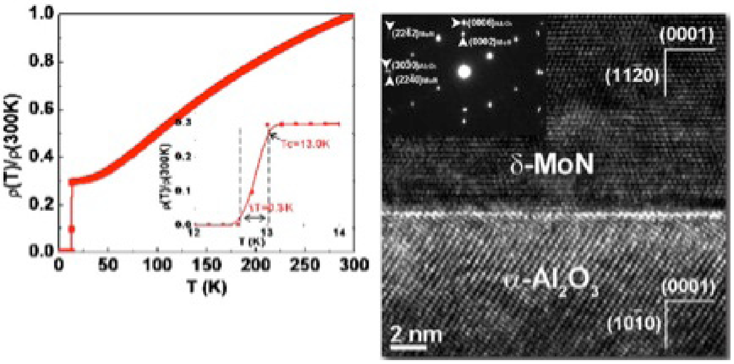
Actinide science is experiencing a renaissance with the emergence of exciting new topical areas, consistent with the importance of actinide materials in modern technological society. As part of the MRS Spring Meeting held recently in San Francisco, Condensed Matter and Magnet Science (MPA-CMMS) researcher Tomasz Durakiewicz organized a symposium on "Actinides – Basic Science, Applications, and Technology." LANL co-sponsored the symposium with Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, and the Institute for Transuranium Elements, Karlsruhe, Germany.

Actinide materials have two main aspects. First, they are technologically and scientifically important. For instance, they form the backbone of technologies for the generation of electricity by nuclear power. Nuclear energy is a long-lasting and powerful energy source, as demonstrated in nature and stars. From a purely scientific point of view, they exhibit fascinating, yet poorly understood, physical and chemical properties. These properties are due in large part to complexities such as f-electron correlations. Second, the toxicity and radioactivity of actinides cause inevitable challenges such as the disposal of nuclear waste. Because radioactive materials pose hazards for humans and the environment, these materials must be well understood to ensure their safe use. Understanding actinide materials is not an easy task due to their complex electronic structures, which push the limits of current theoretical approaches, and the experimental restrictions caused by their toxicity and radioactivity. Even so, great progress in understanding actinide materials is being made.



The symposium brought together those who are studying basic actinide science and those who are developing technological solutions to the challenges posed by actinide materials. The current theoretical and experimental developments and the technological issues of the actinides were presented. Topics included superconductivity and heavy fermions, nuclear magnetic resonance and neutron scattering, novel spectroscopy, 5f-electron chemistry, new materials, and phases, new theory tools, physical properties of transport and magnetism, surface properties and corrosion, environmental effects, radiation damage, nuclear fuels, localization, delocalization, and the dual nature of f-electrons. Jim Boncella (Materials Chemistry, MPA-MC), Steve Valone (Materials Science in Radiation Dynamics and Extremes, MST-8), John Joyce and Georgios Koutroulakis (Condensed Matter and Magnet Science MPA-CMMS), Krzysztof Gofryk (Metallurgy, MST-6), and Rich Martin (Physics and Chemistry of Materials, T-1) each gave an invited talk. Their work supports the Lab's Energy Security, Nuclear Deterrence, and Global Security mission areas and the Materials for the Future science pillar.

Technical contact: T. Durakiewicz



(Left): The epitaxial δ-MoN thin film grown via the polymer-assisted deposition method displays a metallic-like resistivity vs. temperature characteristic above the superconductive transition. The onset of superconducting transition takes place at a temperature of 13.0 K (inset in the left panel). (Right): High resolution transmission electron microscopy (TEM) image taken from the interface between the film and the substrate demonstrates the high epitaxial quality of the δ-MoN on Al_2O_3. The corresponding selected area electron diffraction pattern (inset in the bottom panel) confirms the epitaxial growth of δ-MoN on the substrate.

Epitaxial superconducting δ-MoN films grown by a chemical solution method

The superior mechanical strength, durability, and catalytic activity of transition-metal nitrides compared with many traditionally used metallic elements and/or metal oxides, make metal nitrides attractive for a wide range of technological applications. Moreover, their diverse transport properties (magnetic, semiconducting, metallic, and superconducting) make metal nitrides the choice for the fundamental understanding of multifunctionalities in extreme conditions, such as low temperature and high pressure. Hexagonal molybdenum nitride (δ-MoN) displays the highest superconducting transition temperature (T_c) of the molybdenum nitrides. However, synthesis of pure δ-MoN with the desired superconducting properties usually requires extreme conditions, such as high temperature and high pressure. The difficulty in obtaining pure δ-MoN hinders its fundamental studies and applications. Los Alamos scientists and collaborators from Texas A&M University have developed a chemical solution method, called polymer-assisted deposition, to grow high performance epitaxial δ-MoN thin films on *c*-cut Al_2O_3 substrates at a temperature lower than 900 °C and at ambient pressure. An epitaxial film has a crystalline overlayer on a crystalline substrate of the same structure. The *Journal of the American Chemical Society* has published the research.

The dense, smooth films of δ-MoN prepared via polymer-assisted deposition are phase pure and reveal a T_c of 13.0 K with a sharp transition. The films possess high critical fields (both upper critical field and irreversibility field) and excellent current carrying capabilities, which further prove the superior quality of these chemically prepared epitaxial thin films. The water-soluble polymer used in the polymer assisted deposition process plays crucial roles for achieving the high-quality films. The polymer controls the viscosity of the solution and binds the metal ions to form a homogeneous solution and to prevent premature precipitation of metal ions. The use of a single crystal substrate with crystalline structure similar to the structure of the film allows the heteroepitaxial stabilization of desired phases without the need for extreme process conditions. The successful growth of epitaxial MoN thin films by a controllable and reproducible route enables the study of intrinsic superconducting properties of epitaxial MoN films, which is a significant step toward the applications of superconducting MoN films.

Reference "Epitaxial Superconducting δ-MoN Films Grown by a Chemical Solution Method," *Journal of the American Chemical Society* **133**, 20735, (2011). Researchers include Yingying Zhang (formerly MPA-CINT, currently Tsinghua University, Beijing, China), Nestor Haberkorn (Superconducting Technology Center, MPA- STC), Leonardo Civale and Filip Ronning (MPA-CMMS), Nathan A. Mara, Mujin Zhuo, and Quanxi Jia (MPA-CINT); Karen J. Blackmore, Eve Bauer, Anthony K. Burrell, and Thomas M. McCleskey (MPA-MC); Marilyn E. Hawley (Polymers and Coatings, MST-7); Roland K. Schulze (Metallurgy, MST-6); Tsuyoshi Tajima (Mechanical Design Engineering, AOT-MDE); Haiyan Wang, Li Chen, and Joon Hwan Lee (Texas A&M University).

The research was performed, in part, at the Center for Integrated Nanotechnologies and was funded by the DOE Office of Basic Energy Sciences. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

Technical contact: Quanxi Jia

World record shattered during six-experiment magnetic pulse

Magnet Lab celebration

Researchers at LANL's campus of the National High Magnetic Field Laboratory on March 22 met the grand challenge of producing magnetic fields in excess of 100 tesla, while conducting six different experiments. The hundred-tesla level is roughly equivalent to 2 million times Earth's magnetic field.

"This is our moon shot, we've worked toward this for a decade and a half," said Chuck Mielke, director of the Pulsed Field Facility at Los Alamos.

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Charles Mielke, center, receives congratulations at the moment of the 100-T pulse.

Record… The team used the 100-tesla pulsed, multi-shot magnet, a combination of seven coils sets weighing nearly 18,000 pounds and powered by a massive 1,200-megajoule motor generator. There are higher magnetic fields produced elsewhere, but the magnets that create such fields blow themselves to bits in the process. The system at Los Alamos is instead designed to work nondestructively, in the intense 100-tesla realm, on a regular basis. The Los Alamos facility is one of three campuses forming the National High Magnetic Field Laboratory (NHMFL).

The 100.75-tesla performance produced research results for scientific teams from Rutgers University, École Nationale Supérieure d'Ingénieurs de Caen (ENSICAEN), McMaster University, University of Puerto Rico, University of Minnesota, Cambridge University, University of British Columbia, and Oxford University. The science that we expect to come out varies with the experiment, but can be summarized as:

- Quantum Phase transitions and new ultra high field magnetic states
- Electronic Structure determination
- Topologically protected states of matter.

"Congratulations to the Los Alamos team and our collaborators," said LANL Director Charlie McMillan. "Their innovations and creativity are not only breaking barriers in science, but solving national problems in the process."

See the LANL news release (www.lanl.gov/news/releases/magnetic_field_researchers_target_hundred_tesla_goal.html) for more information.

HeadsUP!

Bike safety

Good weather is here, and more bikers and walkers are out. The Lab's Traffic Safety Committee provides the following reminders:

To cyclists:

- Slow down from high roadway speeds when crossing a bridge or sidepath.
- Set a personal maximum speed of 10 mph in these areas. The sidepath on the Los Alamos Canyon Bridge is about seven feet wide, so in these close quarters you will be overtaking pedestrians with little spare space. When overtaking someone (either cyclist or pedestrian), slow down even further and move to the side of the path away from a cyclist or pedestrian, especially if you are overtaking from the person's rear.
- The use of a bell or other auditory device does not take the place of caution. Sometimes a cyclist ringing a bell or calling out "on your right/left" has resulted in a startled pedestrian (or fellow cyclist) who has behaved unpredictably, especially if lost in their thoughts or their earbuds, which can result in a collision.
- If you are riding on a downhill slope, control your speed unless you are alone on the bridge or sidepath. A high speed collision would be dangerous, not to mention reckless. Riders who want to go fast should take to the roadway.

To walkers:

- Pay attention and walk predictably and to one side or the other. If someone is overtaking you on a bike, don't suddenly change course, because the cyclist may not be able to stop or adjust to your new line.
- Wearing headphones and listening to music makes you less obvious to someone overtaking you and trying to get your attention. It also makes it easier to startle you.

Celebrating service

Congratulations to the following MPA employees celebrating service anniversaries recently:

Mahlon Wilson, MPA-11	20 years
Piotr Zelenay, MPA-11	15 years
Jennifer Martinez, MPA-CINT	10 years
Curtis Osterhoudt, MPA-11	5 years

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To submit news items or for more information contact Karen Kippen, ADEPS Communications Team, 606-1822, or kkippen@lanl.gov.
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